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Avogadro is a molecular editor, designed to be easy to use to construct and view molecules and materials in 3D. It runs on Windows, Linux, and Mac. This manual was largely made on a Mac, but the interface should be very similar on any computer. When you initially open Avogadro you will be presented with a screen such as the one shown below. Opening a File The first thing you will probably want to do is open a file and navigate around the molecule. To do this click on the File menu and select Open.... You can then look through the files on your disk and find an appropriate chemical file. Thanks to Open Babel, a large number of file types are supported including CML, XYZ, SDF, Mol2, PDB etc. Several example molecules are supplied with Avogadro. The screen shot above shows the ethanol.cml file opened up and displayed using the default Ball and Stick display type. Notice that when a new file is opened Avogadro switches from the Draw Tool to the Navigate Tool, which allows you to view the molecule without editing it. You can zoom in/out using the scroll wheel on your mouse or holding down the middle mouse button and moving the mouse cursor up/down. You can rotate the view by holding down the left mouse button and moving the mouse cursor. You can also translate the view by holding down the right mouse button and moving the mouse cursor. Note: if your mouse only has one or two buttons you can also use the modifier keys (shift and control) along with the left mouse button to perform actions where you would normally use the middle or right mouse buttons respectively. Avogadro 2 is currently in beta. It was re-written from scratch to address a number of issues with the Avogadro v1 codebase.Major concerns in Avogadro 1.0 focused on stability (i.e., crashes) and speed, particularly with molecules or systems over a few hundred atoms. Avogadro v2 was designed for fast modern rendering and improved stability. It is a platform to make it easy to build the next generation of molecular and materials visualization and editing tools. A free and open source molecular editor and visualization tool. Designed for students and advanced researchers alike.Used in computational chemistry, molecular modeling, chemistry education, bioinformatics, materials science, and more.Molecules, crystals, biomolecules, surfaces Avogadro loves them all. A sleek interface and user-friendly tools makes working in Avogadro easy, whether you are playing with molecules in 3D for the first time, quickly sketching structures for calculation input, or preparing graphics for publication. With a new, modern 3D renderer, visual effects like reflections and ambient occlusion, and a variety of display options, your molecules look good in Avogadro.A picture paints a thousand words, but a movie tells a story make an animation to bring your chemistry to life. Thanks to the rewritten core and lightning-quick multithreaded renderer, Avogadro 2 handles systems of thousands of atoms effortlessly.Built-in force fields tidy up hand-drawn molecules in seconds. Read your geometry files, wherever they are from Avogadro understands a huge number of file formats, and can write to hundreds.Explore the results of calculations with native output parsing for popular quantum chemistry programs including GAMESS, Gaussian, Molden, MOPAC, NWChem, and ORCA. Plugins add diverse functionality interactive tools, commands, interfaces to other programs, additional force fields and file formats, and more.Writing your own plugin in Python is straightforward.And if its useful, why not share it with the community? Avogadro is free, and all source code and documentation is available under the permissive BSD 3-clause license.Got an issue?The Avogadro community is friendly and ready to help.Got an idea? Development is public and contributions are welcomed. Translations available for Simplified Chinese, English, Esperanto, French, Georgian, German, Hungarian, Japanese, Korean, Portuguese, Romanian, Serbian, and Turkish, with more languages being added all the time. Whether you use Windows, Linux, or macOS to get your work done, Avogadro is available and supported.On ARM?Apple Silicon is already supported, with Windows on ARM a future target.The Qt base means Avogadro looks native and fits right in on your desktop.Get Avogadro Avogadro is an advanced molecule editor and visualizer designed forcross-platform use in computational chemistry, molecular modeling,bioinformatics, materials science, and related areas. It offersflexible high quality rendering and a powerful pluginarchitecture. Cross-Platform: Molecular builder/editor for Windows, Linux, and Mac OS X.Free, Open Source: Easy to install and all sourcecode and documentation is available to modify or extend.International: Translations into Chinese, French, German, Italian,Russian, Spanish, and others, with more languages to come.Intuitive: Built to work easily for students and advanced researchers both.Fast: Supports multi-threaded rendering and computation.Extensible: Plugin architecture for developers, including rendering, interactive tools, commands, and Python scripts.Flexible: Features include Open Babel import of chemical files, input generation for multiple computational chemistry packages, crystallography, and biomolecules.How to cite Avogadro: The Avogadro Paper Avogadro is a free, open source molecular editor and visualizationtool, designed for use on Mac, Windows, and Linux in computationalchemistry, molecular modeling, bioinformatics, materials science, andrelated areas. It offers flexible high quality rendering and apowerful plugin architecture. More about Avogadro, including development details and downloads canbe found at Thanks This book would not be possible without the help and effort of many people, including Avogadro developers, translators, and users world-wide. Funding for the Avogadro manual was provided by the University of Pittsburgh Department of Chemistry. -Taylor Cornell and Geoffrey HutchisonSummer 2015Pittsburgh, Pennsylvania Updated: May 23, 2022 Twitter Facebook LinkedInFrom Avogadro - Free cross-platform molecule editorAvogadro is an advanced molecule editor and visualizer designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It offers flexible high quality rendering and a powerful plugin architecture. Cross-Platform: Molecular builder/editor for Windows, Linux, and Mac OS X. Free, Open Source: Easy to install and all source code is available under the GNU GPL. International: Translations into Chinese, French, German, Italian, Russian, Spanish, and others, with more languages to come. Intuitive: Built to work easily for students and advanced researchers both. Fast: Supports multi-threaded rendering and computation. Extensible: Plugin architecture for developers, including rendering, interactive tools, commands, and Python scripts. Flexible: Features include Open Babel import of chemical files, input generation for multiple computational chemistry packages, crystallography, and biomolecules. How to cite Avogadro: The Avogadro Paper Tell others: . Share the paper We are very proud to announce the availability of Avogadro 1.95.0, the latest Betafor Avogadro 2.0. More can be found on the 1.95 release page including downloads for Mac and Windows. Thanks to many for suggestions, bug reports, and discussions. This release includes many new features, including new protein ribbon / cartoon renderings and the new Layersystem as part of Google Summer of Code by @serk12. Draft developer documentation can be found at If you have comments or suggestions, please join us at and as always, help and contributionsin many forms are very welcome, particularly if youd like to help with user documentation. Features New Layer system, including custom rendering, locking and hiding parts of the molecule @serk12 (#709) Atom and residue labels @serk12 (#715) New protein cartoon / ribbon display @serk12 (#660 #694 #716) Update render options for Wireframe and Ball-and-Sticks @ghutchis (#700 #720) Use MMTF downloads - more efficient than PDB format @ghutchis (#699) Add back support for importing crystals @ghutchis (#658 #659) Add CJSON support for save/load residues and atom colors @ghutchis (#646) Refactor of Python command and input generators, including tabs @ghutchis (#667) New View => Apply Colors menu @ghutchis (#640 #723) Apply color schemes for residues @ghutchis (#638 #688) Add more selection commands, including select by residue @ghutchis (#632 #634) Render selected atoms in VdW and licorice modes @ghutchis (#702) Detect secondary structure from residues / backbones @ghutchis (#685) Save enabled / disabled state of scene / rendering plugins on quit @ghutchis Should now download and install translations for @ghutchis Bug Fixes Fix Mac builds by turning off COORDGEN library @ghutchis (#606) Fix Windows installer to include all needed files @ghutchis Save projection type on close #682 @ghutchis Add a pass to fix OB plugin library paths on Mac @ghutchis (#627 #628) Fix odd behavior on Center command @serk12 (#728) Fix several crashes with proteins @ghutchis (#724 #726 #727) Fix crash in CJSON reading file without labels @ghutchis (#722) Fix bug deleting selected atoms #650 @ghutchis (#672 #677) Fix delete last atom bug @ghutchis (#691) When dragging to create a new atom, use starting coords @ghutchis (#690) Fix #679 - incorrect PDB unit cells @ghutchis (#689) Fixed problems inserting SMILES without coordinates @ghutchis (#661) Fix for transparent widgets @ghutchis (#656) Fix #602 - use Molden order for f-orbitals @ghutchis (#649) If a chain ID is missing / invalid, skip (to read non-standard PDB) @ghutchis (#647) Make sure to reset colors when changing elements @ghutchis (#708) Maintenance Make sure to install crystals directory even when it exists @ghutchis (#613) Replace NULL/0 with nullptr @e-kwsm (#617) Add support for reading partial charge models from obabel @ghutchis (#626) Replace obsolescent LINK_(PRIVATE|PUBLIC) with (PRIVATE|PUBLIC) @e-kwsm (#629) Refactor Molecules class @serk12 (#648) Dont install cclib script - which was removed @ghutchis (#662 #663) Translations Fix fuzzy entry for Nihonium (not Zirconium!) @e-kwsm (#618) Fix all incorrect fuzzy entries #619 @e-kwsm (#643) Remove wrong entries which were fuzzy @e-kwsm (#644) Translations update from Weblate @weblate (#625) Add a workflow which should update the translation template continuously @ghutchis (#624) Thanks to many contributors, including: @12emin34, @GicoProgram, @LihanzUpenn, @NathanBnm, @San4ito, @acunm, @alexrsoares, @danialk03, @dillonschultz93, @e-kwsm, @ghutchis, @grsousajunior, @psavery, @rezaalmanda, @serk12, @tacitcoast, @weblate, Eisuke Kawashima, Jacque Fresco and phlostically If you use Avogadro or Avogadro 2, please consider citing the Avogadro paper: Categories: News Updated: August 16, 2021 Twitter Facebook LinkedIn The latest and greatest release of Avogadro isAvogadro 1.2.0as of 15 June, 2016, and release notes are available. The Avogadro 2 code is a complete rewrite, and can be downloaded here. Avogadro 1 and 2 install to different locations, and can be installed on the same system without issues. You can also download the source code of development branch or stable 1.2.x branch to check out the very latest developments in Avogadro. Windows Linux/Unix Mac Updated: May 23, 2022 Twitter Facebook LinkedIn 21 January 2025New rendering options, including depth-of-field blur and fog from @perminder-17Faster surface mesh generation using the flying edges algorithm @perminder-17Brought back the molecular orbitals panel @ghutchisSupport for translucent balls-and-sticks, van der Waals spheres, and licorice rendering including per-layer customization @ghutchisNew, improved Flatpak package from @matterhorn103 including support for ARMNew conformer properties window @ghutchisNew improved molecular properties window, including charge and spin multiplicity, HOMO and LUMO energies, total energies and other properties (depending on file format) @ghutchisMany more properties parsed from ORCA output files including Hirshfeld, MBIS, and CHELPG charges @ghutchisCode signing on Windows to minimize Defender warnings @ghutchis thanks to SignPathSupport for latest Qt6 on Linux @matterhorn103Improved spectra plots, including NMR, UV and CD spectra (#1874)Add support for reading and rendering DNA / RNA backbones (#1831)Improve python selection dialog (#1844)Calculate and render dipole momentsEdit molecule name, charge, and spin in properties (#1810)Improve manipulate dialog - rotate around origin, molecule center, selection center (#1774)Update the template tool to place ligands or functional groups (#1777)Support for additional secondary structures (3-10 and pi helix) @TactfulDeity (#1746)Implement g orbitals (#1826)cp2kinput improvements @e-kwsm (#1702)Add support to render atomic partial charge labels (#1726)Add support to render bond lengths (#1871)Add HOMO and LUMO energies to molecular properties (#1803)Add Shortcut Keys to navigate/modify tools (Issue #1794) @Milziade (#1807)Add change elements dialog (#1863)Editing molecular charge / spin => input generators and pluginsParse inputParameters if present in cjson (#1849)Read radicals from SDF / Molfile (#1848)Parse more MOPAC aux properties including coordinates (#1843)Parse CHELPG charges from ORCA output too (#1829)Export to XYZ format with 10 decimal precision as per forum debate (#1824)Read MBIS charges from ORCA output (#1823)Read multiple ORCA coordinate sets (#1808)Parse NMR spectra from ORCA (#1799)Parse ORCA electronic spectra (#1797)Add basic support for v3000 molfiles, including for large molecules (#1765)Small patch to parsing XYZ trajectories to handle ORCA 6 separators (#1705)Add support for reading and writing atom force vectors (#1674)Support reading files in UTF-16 formatAllow surface generation to be cancelled (#1894)Add progress bar for optimizations, including cancel (#1893)Switch text rendering to use interpolation (#1917)Fix code for haptic ligands. Pick the furthest dummy to attach (#1916)Only enable the PQR search command if the site is reachable (#1892)Tweak the centroid and center-of-mass commands (#1891)Fix manipulate and label tools to rotate by default (#1861)Fix right-click to delete a hydrogen and adjusting after deleting a bond (#1896)Copy bonds and bond orders when generating super cells (#1898)Fix parsing molecular orbital coefficients in some ORCA output files (#1899)Handle upper-case [ATOMS] line in Molden files from Cfour (#1785)Fix plugin downloader @matterhorn103 (#1767)Prevent a possible unhandled exception from parsing JSON (#1742)Fix crash when creating ligands from the clipboard off-by-one bug (#1739)Ensure BABEL_LIBDIR and BABEL_DATADIR are set properly on Mac (#1736)Fix XYZ trajectories - prevent final frame with 0,0,0 coords (#1720)Make sure the measure tool has a good contrast with background color (#1718)Switch import format for Open Babel to CJSON if supported (#1707)Fix perception of amide nitrogens - should be sp2-like (#1652)Default tool wasnt set properly, so rotations, etc. ignored (#1647)Add more error checking for Fetch PDB (#1646)Fix bug reported in #1637 with mis-parsing selenium atoms in PDB (#1643)Ask before re-perceiving a space group (#1639)Switch back to importing from PDB using PDB instead of MMTF format (#1642)Fix crash with short TER record (#1640)Fix crash when reading cjson with invalid layer data (#1636)Fixed Select bugs reported on forum (#1625)Fix crash from centroids with empty molecule (#1624)Fix crash at startup when opening a file from command-line (#1621)Fix drag-to-install for scripts, esp. energy calculatorsApp crashes when clicking Optimize Geometry without any atom @perminder-17 (#1661)Clarify line width / size in spectra dialog (#1678)Add double-check for addEdge to prevent potential crash (#1704)Ensure split buttons dont create a transparent backgroundUse QDesktopServices on Linux too with Qt 6, which fixes opening URLs @matterhorn103Update desktop file name in QApplication code @matterhorn103Update the newer compilation guide @nbehrndExport icons according to XDG icon spec on unix @matterhorn103Use name according to the XDG standard, harmonize metadata with flatpak @matterhorn103Make sure to create directories for drag-and-drop install of Python scriptsTweak the text and tooltips in the rendering dialogFix crash when no selection is made when saving filesUse flying edges for mesh generation @perminder-17 (#1741)When possible, load Python script names from cache (#1830)Turn off default depth blur, shadows, edge for speed (#1728)Updated tests to Qt6 @peach280 (#1941)Explicitly use signed char in meshgenerator to avoid narrowing error on ARM @matterhorn103 (#1842)Fix residue not initializing id in default constructor (#1786)ENH/BUG: Code Clean Up, Optimization, Documentation @TactfulDeity (#1779)Add flatpak workflow for GitHub Actions @matterhorn103 (#1772)Update to latest Qt patch version and install-qt-action @matterhorn103 (#1841)Set a project-wide variable for molecule data dir AvogadroLibs_SOURCE (#1851)Unbundle all charge and forcefield scripts (#1832)Update comment headers to new format (missed some in prev effort) (#1828)Use release certificate signing on Windows (#1821)Bumping to Qt 6.8 (latest LTS) for Mac and Windows builds (#1751)Switch AppImage build to use the new linuxdeploy tool (#1775)Further fixes for Qt6 @matterhorn103 (#1713)Fix building Qt Plugins without spglib (USE_SPGLIB=OFF) @MehdiChinoune (#1671)Cmake: Remove custom Find.cmake modules @LecrisUT (#1585)Fix wrong variable name @antonio-rojas (#1612)Fix windows debug logRemove many incorrect fuzzy translations @e-kwsmFix a few ellipsis inconsistencies @matterhorn103 (#1771)chore: put space after period @e-kwsm (#1697)Automated translation updates @github-actionsTranslations update from Hosted Weblate @weblate Thanks to many contributors, including: @Cartrigger, @LecrisUT, @MehdiChinoune, @Milziade, @NorwayFun, @RickyLam11, @SantosSi, @TactfulDeity, @TamilNeram, @ZhangHMDS, @alexrsoares, @andibing, @antonio-rojas, @dependabot, @e-kwsm, @ghutchis, @github-actions, @matterhorn103, @milotype, @nbehrnd, @ostriz2, @ovari, @peach280, @perminder-17, @rezaalmanda, @secretkontributer, @simmon-nplob, @snowcliffx, @tacitcoast, @weblate, @ykertytsky, @zhangtengshuo, Eisuke Kawashima, KeysBits, LibreTranslate, Remus-Gabriel Chelu, Weblate Translation Memory, fox and gallegonovato 10 February 2024Further improvements to the new optimization framework, including default integrated Open Babel force fields (MMFF94, UFF, GAFF)New toolbar icons with light / dark theme from @matterhorn103Significantly faster molecular and orbital surfacesVibrational spectra plottingSupport for installing Python packages with plugins via pip or condaImproved selection of conda environmentsConformer search dialog through Open BabelImproved template tool for inserting ligands and functional groupsSignificant improvements from @nbehrnd for the ligand libraryLogging debugging / error messages to a file for Windows usersAdd optional energy / optimize code that links Open Babel @ghutchisUpdate tool plugins to set icon as light / dark theme @ghutchisModern tool icons @matterhorn103Add confirmation dialog to install with conda or pip @ghutchisAdd support for first launch dialog and conda environments @ghutchisAdd red = a, blue = b, green = c color axes for unit cells @ghutchisVibrational spectra plot @ghutchisAdd UniqueID atom label type @ghutchisAdd ethylene, ethyne, and phosphate standard functional groups @ghutchisImproved python configure dialog @ghutchisAdding support for bond label in base classes and CJSON @ghutchisAdd indicator for display types with settings @ghutchisSplit ligands and functional groups in the template tool @ghutchisAdded copy and export feature to property tables @Surajjalpun2002Add initial support for copy from tables @ghutchisAdd conformer search box @ghutchisAdd template library to insert ligands or functional groups @ghutchis (#1456)Add support for Hall number and space group to CJSON read/write @ghutchis (#1440)Add new MessagePack version of CJSON @ghutchis (#1452)Add a message handler to grab debug / warnings on Windows @ghutchisSave and load the camera modelView and projection matrix @ghutchisFixed typo in setDefaultPythonInterpretor() @matterhorn103 (#1583)Fix Mac builds @ghutchis (#1522)Fix quantum surface max cutoff for diffuse functions @ghutchis (#1556)Change Insert fragment Insert molecule by popular request @ghutchis (#1519)Fix parsing XYZ files with tabs between columns @ghutchis (#1513)Fix bug with incorrect Unicode characters added to labels @ghutchis (#1588)Fix for Wayland @matterhorn103 (#1577)Fixed crash with angle properties on an empty molecule @secretkontributer (#1566)Fix density color crash @ghutchis (#1537)Fix crash in forcefields - check if method is valid before using it @ghutchis (#1526)Fix for first item in ordered plugin dialog being empty @matterhorn103 (#1523)Fix crash with copy as and an empty molecule @ghutchis (#1521)Turn off Color Opacity Map unless a VTK widget is active @ghutchis (#1509)Make sure to automatically load the Meshes display type @ghutchis (#1508)If no partial charges are assigned, set them @ghutchis (#1502)Fix potential crashes in selection commands @ghutchis (#1499)Fix vibration animation @ghutchis (#1487)Generate the density matrix if needed for the electron density surface @ghutchis (#1482)Fix empty window showing up for commands without an option dialog @ghutchis (#1468)Save partial charges and properly read them from CJSON @ghutchis (#1467)Dont show PNG files in the filter dialog @ghutchis (#1462)Fix GFN-FF energy - redirect GFN-FF output through a hack @ghutchis (#1454)Fixup PDB reading with non-standard MD files (no element column) @ghutchis (#1450)Fix atomic numbers from Orca - it would read electrons not symbols @ghutchis (#1451)Fix linear molecular template @ghutchis (#1474)Avoid segfaulting while manipulating carbon bonds/hydrogens @Makiah (#1493)Reduce ambiguity of Export toolbar button @matterhorn103 (#442)Ensure that title bar correctly displays active molecule file @Makiah (#440)Allow scripts to add properties (orbitals, vibrations, cubes) @ghutchisAdd support for navigator commands - rotate, translate, zoom @ghutchisWindows: Standardize plugin location based on forum feedback @ghutchisAdd some additional Python classes including cjson and connect @ghutchisAlways supply cjson to scripts @ghutchisIf userOptions specifies an order, use that to sort the form @ghutchisCheck script menupath for {} priority numbers @ghutchisAdd a text option for scripts to add text labels / help @ghutchisSkip calculating orbital / surface points too far apart (e.g., negligible) @ghutchisLeads to 2-3x faster surface generationPackage OpenSSL for Windows @ghutchisUpdate Eigen cmake header references @ghutchis (#1544)Add Qt6 build tests @ghutchis (#1547)Update to cibuildwheel for Python 3.12 @ghutchis (#1546)Fix include of avogadrocoreexport.h @ghutchis (#1504)Add specialization for char* and MatrixXf types @ghutchis (#1494)Install ligand and functional group fragments @ghutchis (#1460)Make sure to copy libopenbabel on Mac for CPack @ghutchisCorrect typo @Acylation (#1553)Update Australian and Canadian localization from GB version @ghutchis (#1453)Translations update from Hosted Weblate @weblateAutomated translation updates @github-actionsFix a few remaining cases of instead of ellipsis character @ghutchis (#1458) Thanks to many contributors, including: @Acylation, @Azaathooth, @IagoEmanuel15, @ImgBotApp, @Makiah, @NorwayFun, @Surajjalpun2002, @alchemistcai, @bitigchi, @dependabot, @dependabot[bot], @ghutchis, @github-actions, @hakkikonu, @imgbot, @imitrichev, @joerivan, @koenr, @matterhorn103, @nbehrnd, @ovari, @research11111, @secretkontributer, @tacitcoast, @weblate, Alejandro Daz-Moscoso, Eisuke Kawashima, Ivanushka, LibreTranslate, Remus-Gabriel Chelu, Weblate Translation Memory and gallegonovato

Illustrate avogadro's number with examples. Differentiate between mole and avogadro's number with examples. Avogadro's number derivation. Avogadro's number and atomic weight. Avogadro's number practice problems. Define and explain mole and avogadro's number with examples. What are avogadro's number. Avogadros konstant.

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